

chain nodes:

21

ring nodes:

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 22 23 24 25 26

chain bonds:

5-7 6-8 21-22

ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6 7-9 7-13 8-14 8-18 9-10 10-11 11-12 12-13 14-15 15-16 16-17 17-18 22-23 22-26 23-24 24-25 25-26

exact/norm bonds:

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-8 21-22 22-23 22-26 23-24 24-25 25-26

normalized bonds:

7-9 7-13 8-14 8-18 9-10 10-11 11-12 12-13 14-15 15-16 16-17 17-18

G1:C,N

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 21:CLAS\$22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom